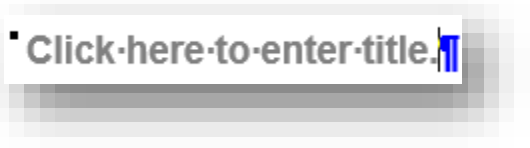
LEIS Template Instructions

Guide to using this Template

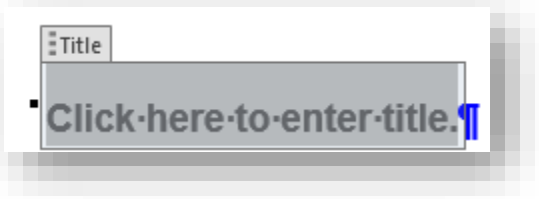
For ease-of-use, this template has been designed as a Microsoft Word form that when filled, will closely resemble a published ***Surface Science Spectra*** article. Authors are encouraged to consult published articles for additional guidance. The form consists of two types of fields: standard and drop down.

Standard Fields

To enter content into a standard field, click on the grey field instructive label.



The field will open and content can be added either by typing directly, or by copy/paste from another document.



Drop-down Fields:

To choose content from a drop-down field, click on the grey field instructive label.

The field will open and content can be chosen from the menu by clicking on the appropriate item.

Figures:

A key feature of ***Surface Science Spectra*** is the uniformity of its figures. As such, SSS adheres to strict figure formatting guidelines (described below). Figure production templates are available for Origin and Excel. For more information of figure formatting, see Appendix A and B of this document.

Initial submission process: Authors may copy/paste (as a picture) spectra into the appropriate spectrum placeholder as indicated. Leave the "Accession #" label shown in the figure template as is during this phase. Unique accession numbers will be assigned to each specimen in the submission once the manuscript has been accepted. The accession number(s) will be sent to the authors to add to the final versions of the figures.

Final submission process: Authors need to send each figure (as a separate file) in one of the following formats: PostScript (.ps), Encapsulated PostScript (.eps), TIFF, or production-ready PDF. You can name each Figure file with a descriptive title such as Figure1, Figure 2, etc.

Instructions for Origin and Excel:

Font sizes:

1. Accession# label inside plot is **Arial 16 bold**.
2. Axis labels are Arial 14.
3. Tick labels are Arial 11.
4. Peak labels are Arial 11.

Plotting:

Templates are available for producing properly formatted SSS figure with Origin or Excel. Workbooks contain worksheets and plots for the spectra. Authors need only replace the existing (x,y) data with the data to be plotted. To add additional figures using Origin, create a new worksheet, right-click on the header of the appropriate spectrum type, select duplicate (batch plotting), select the new worksheet, press ok, and then add the data to be plotted to the new worksheet. To add additional figures using Excel, right-click on a bottom worksheet tab, select move or copy, choose the sheet of the appropriate spectrum type, click create a copy, press ok, and then replace the existing data in the new worksheet with the data to be plotted.

Labelling:

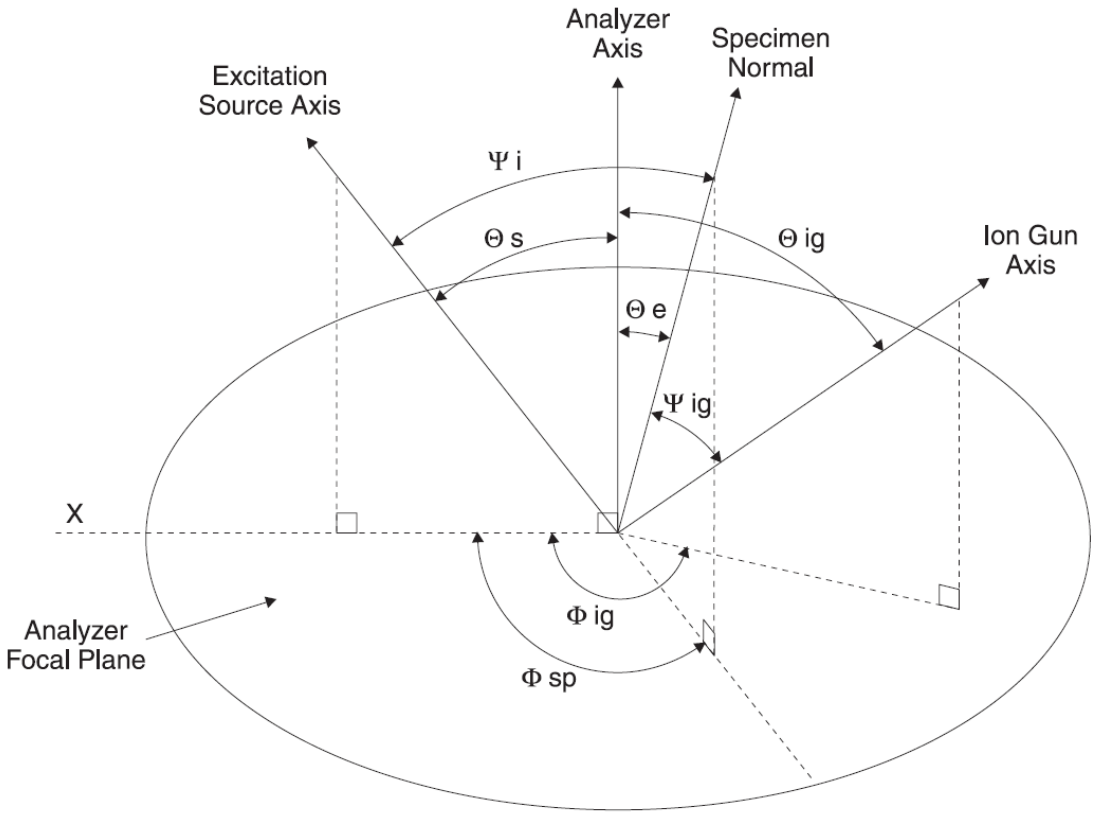
Additional labelling of the figures can be done directly using Origin. Additional labelling of the figures can be done using PowerPoint. To create figures for production, define the slide area as 8.5 x 11 portrait mode and then copy/paste each figure on individual slides.

Data files

Please submit your spectra as tab-delimited x,y ASCII datasets (*.asc) with headers indicating the content of the column (*i.e.* Binding energy or Kinetic energy and counts or counts/s).

Spectrometer Geometry Diagram and Worksheet

The spectrometer geometry is specified with respect to a coordinate system in which the axis of the analyzer defines the polar (Z) axis, and the X-Y axes lie in the analyzer focal plane. The X axis is defined by the normal projection of the excitation source axis onto the analyzer focal plane. If the analyzer and source axes are coincident, the projection of the ion gun onto the focal plane should be used as the azimuthal reference. Another reference may be more convenient. Describe your choice of reference in Section C, Field 20 on the previous page. It is presumed that all component axes intercept at a common point lying on the specimen surface.



Field Name	Label	Value* (in degrees)
Emission Angle	Θ e	
Incident Angle	Ψ i	
Source-to-Analyzer Angle	Θ s	
Specimen Azimuthal Angle	Φ sp	
Sputter Source Incident Angle	Ψ ig	
Sputter Source Polar Angle	Θ ig	
Sputter Source Azimuthal Angle	Φ ig	

Submission Overview

Title: Enter title, beginning with a descriptive reference to the specimen material or other characteristics specific to this data record. Avoid titles which begin with the technique, such as 'AES Study of....'

Authors: Enter authors names as you wish them to appear in *SSS*.

Affiliations: Enter authors' affiliations as you wish them to appear in *SSS*.

Abstract: Summarize and include key information about the specimens and spectra, such as specimen material, measurement procedures, and significance of the research. The abstract will be printed verbatim. Because the abstract must stand alone in some databases, **please do not cite references in the abstract**. You may include references in the **Introduction**, below.

Keywords:

Technique: (drop down with choices –LEIS, HS-LEIS) Choose the spectroscopy technique used.

Host Material: Provide a generic description of the specimen, such as nylon, 6061 Al, or SiO_2. For layered structures, the host material is the 'bulk' substance near the surface.

Manufacturer and Model: Enter the instrument manufacturer name. If the instrument was custom-built, enter the designer's name and reference a published article, if applicable. Enter the manufacturer's model number.

Major Elements in spectra:

Minor Elements in spectra:

Published Spectra: Enter the number of specimen and calibration spectra for which you are requesting hard-copy publication. An opportunity to identify specific spectra for publication is given in the template figure caption. For datasets that you do not wish to publish the spectra, but wish to make available to the readers, please contact the AVS Publications Office for more information.

Spectral Category: Choose the suggested category of the data record **drop down with choices: Technical**, **Comparison**, or **Reference** (see overview of instructions for definitions). The editors may suggest an alternate category, based on the recommendations of referees.

Introduction

Enter any descriptive, explanatory or introductory comments that pertain to your entire submission, *e.g.* why the work is significant, or what the conclusions show. You may cite references.

Specimen Description

Note: Multiple specimens may be included in a single SSS submission. To add additional specimens, copy/paste the entire 'Specimen Description' section (including the header), placing the new sections in the order you would like to have them appear in the final publication.

Accession number: Replace "00000" with a single letter for initial submission. *i.e.* "A", "B", "C", … (Select A for the first specimen and continue alphabetically for subsequent specimens). Note that this letter should also be implemented in the figure file, data file, and spectral ID as per the *Information for Contributors* document.

Host Material: Provide a generic description of the specimen, such as nylon, 6061 Al, or SiO_2. For layered structures, the host material is the 'bulk' substance near the surface.

Chemical Abstract Service (CAS) Registry #: Enter the CAS registry number of the host material. Enter 'unknown' if not known.

Host Material Characteristics: Homogeneity: (drop down with choices – Homogeneous, Inhomogeneous, Unknown), choose the one that best applies. **Phase:** (drop down with choices – Gas, Liquid, Powder, Solid), **c**hoose the one that best applies. **Crystallinity:** (drop down with choices – Amorphous, Polycrystalline, Single Crystal, Unknown Crystallinity), **c**hoose the one that best applies. **Electrical Characteristics:** (drop down with choices – Conductor, Dielectric, Semiconductor, Superconductor, Unknown Conductivity), choose the one that best applies. **Material Family:** (drop down with choices – Biological Material, Composite, Inorganic Compound, Metal, Organic Compound, Polymer,

Semiconductor), choose the one that best applies. **Special Material Classes:** (drop down with choices – Ceramic, Coating, Fiber, Glass, Other, Powder, Thin Film, nanoparticles), choose all appropriate responses. Leave blank if Special Classes do not apply. If 'Other,' describe in 'As Received Condition' (copy/paste this field as necessary).

Chemical Name: Enter the full chemical name of the host material according to IUPAC conventions, *e.g.* for Li_3PO_4 you would enter lithium orthophosphate.

Source: Provide the name of the manufacturer and/or supplier of the host material, or give a reference to how the host was made, *e.g.* thermally grown SiO_2 on Si.

Lot Number: Provide the code that identifies the production run, etc.

Host Composition: List the principal elements present or the chemical formula, if practical.

Form: Give a physical description of the host, *e.g.* MOSFET, reagent, single-crystal wafer, stub from corroded fender from brand X pickup truck, etc.

Structure: Include information such as a description of the crystal lattice and orientation, *e.g.* [1 0 -1 0] hexagonal close-packed, and/or comments such as fracture surface at grain boundary, etc. You may also submit a hard-copy bonding diagram.

History and Significance: Comment field for background information about the specimen, *e.g.* moon rock retrieved by Apollo IX mission, or a discussion of why the spectra were taken. Include comments on purity, known contaminants, results of other analytical techniques. Identify the organization that developed any specified alternate standard designator, *e.g.* AISI in the case of 1003 carbon steel.

As Received Condition: Describe the physical condition of the specimen as it was supplied to the spectroscopist, *e.g.* as grown, paint delaminating from metal stub, etc. Include the thermal and storage history of the specimen as well as physical condition.

Analyzed Region: Describe the specimen analyzed qualitatively, *e.g.* shorted FET gate, same as host material, or weld bead.

Ex Situ Preparation and Mounting: Describe specimen preparation prior to introduction into the spectrometer vacuum system, *e.g.* as received, washed in ethanol, scraped with a well-pickled file, etc. Also, describe the specimen mounting technique.

In Situ Preparation: Describe specimen preparation or treatment procedures within the spectrometer vacuum system prior to analysis, *e.g.* ion sputter cleaning and annealing.

Charge Control Conditions and Procedures: Describe the equipment used to control charge of the specimen during measurement. Include flood gun voltages and current, target bias, the use of metal screens, etc. Also describe the procedures used to determine the charge control.

Temperature During Analysis: Enter the specimen temperature during analysis, in Kelvin. Use 300 for 'room temperature' if not otherwise measured.

Pressure During Analysis: Enter the maximum chamber pressure during analysis, in Pascal (1 Torr = 133 Pascal). Normally you would express this using powers of 10, for example $1.33x10^{-6}$.

Partial Pressure of Reactive Gases) During Analysis: Enter the partial pressures of reactive gases in the chamber if they have been used during analysis, in Pascal.

Reference Sample for Quantification

Chemical Name: Enter the full chemical name of the host material according to IUPAC conventions, *e.g.* for Li_3PO_4 you would enter lithium orthophosphate.

Source: Provide the name of the manufacturer and/or supplier of the host material, or give a reference to how the host was made, *e.g.* thermally grown SiO_2 on Si.

Homogeneity: (drop down with choices – homogeneous, patterned, inhomogeneous)

Form: Give a physical description of the host, *e.g.* MOSFET, reagent, single-crystal wafer, stub from corroded fender from brand X pickup truck, etc.

Specific Surface Area: Enter the specific surface area, in m^2/g.

Comment: Comment field for background information about the reference sample.

Ex Situ Preparation and Mounting: Describe specimen preparation prior to introduction into the spectrometer vacuum system, *e.g.* as received, washed in ethanol, scraped with a well-pickled file, etc. Also, describe the specimen mounting technique.

In Situ Preparation: Describe specimen preparation or treatment procedures within the spectrometer vacuum system prior to analysis, *e.g.* ion sputter cleaning and annealing.

Charge Control Conditions and Procedures: Describe the equipment used to control charge of the specimen during measurement. Include flood gun voltages and current, target bias, the use of metal screens, etc. Also describe the procedures used to determine the charge control.

Temperature During Analysis: Enter the specimen temperature during analysis, in Kelvin. Use 300 for 'room temperature' if not otherwise measured.

Pressure During Analysis: Enter the maximum chamber pressure during analysis, in Pascal (1 Torr = 133 Pascal). Normally you would express this using powers of 10, for example $1.33x10^{-6}$.

Partial Pressure of Reactive Gases) During Analysis: Enter the partial pressures of reactive gases in the chamber if they have been used during analysis, in Pascal.

Instrument Description

Manufacturer and Model: Enter the instrument manufacturer name. If the instrument was custom-built, enter the designer's name and reference a published article, if applicable. Enter the manufacturer's model number.

Analyzer Type: (drop down with choices – Cylindrical Mirror, Double Toroidal, Spherical Capacitor, Time-of-flight, other) Choose the analyzer type that best applies. If 'other,' include a description.

Detector: (drop down with choices – channeltron, dynode, multichannel resistive plate). Describe the detector used.

Number of Detector Elements: Enter the number of detector elements. For a multichannel detector, this would be the number of separate detector data channels that can be output (*e.g.* 3, 5, 16, 128). For a single-channel detector, the number is '1.'

Instruments Parameters Common to all Spectra

Spectrometer

Analyzer Mode: (drop down with choices – Constant Pass Energy, Constant Retarding Ratio option) Choose **Constant Pass Energy** (fixed analyzer transmission) or **Constant Retard Ratio**, whichever best applies.

Energy Dependence of Detection: (drop down with choices – constant, proportional, higher order) Identify the energy dependence of detection. Choose from constant, proportional, higher order.

Charge Compensation Energy: Enter the charge compensation value in eV.

Time of Flight Filter Used: (drop down with choices – yes, no). Indicate whether a time of flight filter was used.

Time of Flight Filter Comment: Enter time of flight filter comment.

Ion Sources

***Ion Source 1 of** Enter number of ion sources used.*

Purpose of this Ion Source: (drop down with choices – analysis beam, sputtering beam, other) Indicate the purpose of the ion source. Choose from analysis beam, sputtering beam, other.

Manufacturer and Model: Enter the ion gun manufacturer, or describe as completely as possible if non-standard. Enter the ion gun model, if applicable.

Energy: Enter the ion energy in eV.

Current: Current value: Specify the ion current in either total current to specimen (units in mA or equivalent) or current density to unit area of the specimen (mA/cm^2). **Current Units: (drop down with choices – mA, mA/cm^2).**

Current Measurement Method: (drop down with choices – Biased Stage, Faraday Cup option) Choose the one that best applies.

Species (drop down with choices – 3He, 4He, 20Ne, 40Ar, 84Kr). If you are using a primary beam species other than the choices, please enter the primary beam species name.

Spot Size (unrastered): Define the full-width-half-maximum (FWHM) diameter of the (unrastered) ion gun beam in micrometers as measured normal to the ion gun axis.

Raster size: X-raster value. Use the x and y deflection electrodes of the ion gun to define the axes. Measure in μm. Y-raster value. Use the x and y deflection electrodes of the ion gun to define the axes Measure in μm.

Incident Angle (Ψ ig):

Scattering (Polar) Angle (Θ ig):

Azimuthul Angle (Φ ig):

Comment: List any comments to help understand the sputtering procedure, such as equivalent silicon dioxide sputter rate, crater flatness, etc. State whether sputtering was performed with a differentially pumped ion gun or by backfilling the chamber**.**

Data Analysis Method

Energy Scale Correction: Discuss energy scale calibration and energy shift used to compensate for charging, if any.

Peak Shape and Background Method: Describe background correction technique, *e.g.* linear subtraction, Shirley function, Tougaard function, Fourier transform cutoff, etc. Describe the procedure used to fit the spectral line shape, *e.g.* Gaussian, Lorentzian, Voight, etc.

Quantitation Method: Specify the method used to determine the values for the atomic concentrations for the analyzed region. Please cite references for the quantitation method in the References section.

Sensitivity Factor (source): Enter the source, or method of determination, of the sensitivity factor(s).

Acknowledgments

Acknowledgments to be published in *Surface Science Spectra.*

References

References to be published in *Surface Science Spectra*.

Spectral Features Table

Spectrum ID#: The official ID number will be assigned to you on acceptance. For initial submission, please enter the first part of the data (X,Y) file name (minus the extension), in the rows that relate to that file. Note: There are instructions on the required file naming scheme for initial submission found in *Information for Contributors*.

Peak Energy: Enter the peak energy, in eV, used to fit this spectral peak component.

Peak FWHM: Enter the full width at half maximum (FWHM), in eV, used to fit this spectral peak component.

Peak Area: Enter the peak amplitude for this spectral peak. Units are as specified in the Peak Amplitude Units field. **Peak Amplitude Units: (drop down choice – cts/nC, counts/sec, eV x counts, eV x counts/sec, normalized to a selected peak intensity, total counts)** No instructions

Sensitivity Factor: Enter the sensitivity factor used in quantitation for this peak.

Concentration: Enter the concentration for this peak.

Concentration Units: (drop down choice – atomic percent, mg/m^2, monolayers, other, weight percent). No instructions

Primary Ion Species: Enter the name of primary ion species used for each spectrum.

Peak Assignment: Enter a brief identification of the peak assignment, *e.g.* carboxylate, Mo(IV), C in C-O, etc.

Comments to Spectral Features Table: Enter any comments or additional information as a footnote to this table pertaining to the entire Spectral Features Table.

Peak Comment: Enter any brief comment as a footnote to this table regarding this peak, *e.g.* 'Concentration includes both lattice oxygen and adsorbed oxygen,' or 'Labeled V'' in figures,' or 'The bulk PVC samples were contaminated with small amounts of Si and O.'

Guide to Figures

Spectrum ID#: The official ID number will be assigned to you on acceptance. For initial submission, please enter the first part of the data (X,Y) file name (minus the extension), in the rows that relate to that file. Note: There are instructions on the required file naming scheme for initial submission found in *Information for Contributors*.

Spectral Region: Enter the element(s) corresponding to this spectrum.

Voltage Shift: Enter the number which, when subtracted from the corrected abscissa value, will yield the original abscissa value (*i.e.* the opposite of the value(s) given in the **Recommended Energy-Scale Shift field**).

Multiplier: Enter the multiplier (scaling factor) applied to the ordinates values of the spectrum. Enter 1 if no multiplier was applied.

Baseline: Enter the baseline offset that was applied to the ordinates values of the spectrum. Enter 0 if no offset was applied.

Comment: Enter any brief comment regarding this spectrum.

Spectra

Paste the spectrum, as you would like it published including all peak labels, into the appropriate place-holder. SSS will publish plots of corrected data, but please indicate explicitly whether the submitted plotted data represent raw or corrected data. Curve fits will always be plotted on top of the raw (or shifted) data, NOT against background-subtracted data. Authors must provide digital curves representing all components of the fit, including any background subtraction. Preferred file formats for plots are PostScript (.ps), Encapsulated PostScript (.eps), TIFF, production-ready PDF or JPG.

Spectrum Figure Caption

Host Material: Provide a generic description of the specimen, such as nylon, 6061 Al, or SiO_2. For layered structures, the host material is the 'bulk' substance near the surface.

Technique: (drop down with choices –LEIS, HS-LEIS) Choose the spectroscopy technique used.

Spectral Region: Enter the spectral region for this energy range.

Instrument: Enter the instrument manufacturer name. If the instrument was custom-built, enter the designer's name and reference a published article, if applicable. Enter the manufacturer's model number.

Primary Ion Energy (eV): Enter the ion energy in eV.

Primary Ion Species (drop down with choices – 3He, 4He, 20Ne, 40Ar, 84Kr). If you are using a primary beam species other than the choices, please enter the primary beam species name.

Primary Ion Fluence: Specify the primary ion fluence in ions/cm^2.

Analysis Field of View: Enter the X and Y values, in mm, of the analyzer field of view. Choose X and Y axes to correspond with the manufacturer's definitions. In choosing the axes, insure that X and Y are orthogonal to each other and to the analyzer axis.

Analyzer Type: (drop down with choices – Cylindrical Mirror, Double Toroidal, Spherical Capacitor, Time-of-flight, other) Choose the analyzer type that best applies. If 'other,' include a description.

Analyzer Type: (drop down with choices – CMA, DCMA, Other-describe in next field, SSA) Choose the analyzer type that best applies. If 'Other,' include a description in 'Non-Standard Analyzer or Lens'.

Incident Angle (Ψ i):

Scattering (Polar) Angle (Θ ig):

Analyzer: drop down with choices - retarding ratio or the pass energy in eV. **Analyzer Constant:** Enter analyzer constant value.

Analyzer Resolution: Enter the analyzer resolution, in **%** if the analyzer is operated with a constant retarding ratio, or in **eV** for constant pass energy analyzers

Total Signal Accumulation Time (sec): Enter the time, in seconds, spent accumulating data into displayed channels.

Total Elapsed Time (sec): Enter the time, in seconds, to complete the acquisition of the spectral data. The total elapsed time includes the Signal Accumulation time (previous field), the settling time, and the overscan time.

Number of Scans: Specify the number of times the signal for a given channel was counted.

Effective Detector Width (eV): Enter the detector width. For a multichannel detector, this would be the width, in eV, of the portion of the spectrum acquired simultaneously by the detector. (In a case where the effective width may vary with energy across the spectrum due to the type of analyzer used, an average detector width may be used, with the behavior described more fully in the 'Detector Description' in Section C.) For a single channel detector, the width can be listed as the eV/step in the spectral data.

Reference Spectrum (Optional) Figure Caption

Host Material: Provide a generic description of the specimen, such as nylon, 6061 Al, or SiO_2. For layered structures, the host material is the 'bulk' substance near the surface.

Technique: (drop down with choices –LEIS, HS-LEIS) Choose the spectroscopy technique used.

Spectral Region: Enter the spectral region for this energy range.

Instrument: Enter the instrument manufacturer name. If the instrument was custom-built, enter the designer's name and reference a published article, if applicable. Enter the manufacturer's model number.

Primary Ion Energy (eV): Enter the ion energy in eV.

Primary Ion Species (drop down with choices – 3He, 4He, 20Ne, 40Ar, 84Kr). If you are using a primary beam species other than the choices, please enter the primary beam species name.

Primary Ion Fluence: Specify the primary ion fluence in ions/cm^2.

Analyze Field of View: Enter the X and Y values, in mm, of the analyzer field of view. Choose X and Y axes to correspond with the manufacturer's definitions. In choosing the axes, insure that X and Y are orthogonal to each other and to the analyzer axis.

Analyzer Type: (drop down with choices – Cylindrical Mirror, Double Toroidal, Spherical Capacitor, Time-of-flight, other) Choose the analyzer type that best applies. If 'other,' include a description.

Analyzer Type: (drop down with choices – CMA, DCMA, Other-describe in next field, SSA) Choose the analyzer type that best applies. If 'Other,' include a description in 'Non-Standard Analyzer or Lens'.

Incident Angle (Ψ i):

Scattering (Polar) Angle (Θ ig):

Analyzer: drop down with choices - retarding ratio or the pass energy in eV. **Analyzer Constant:** Enter analyzer constant value.

Analyzer Resolution: Enter the analyzer resolution, in **%** if the analyzer is operated with a constant retarding ratio, or in **eV** for constant pass energy analyzers

Total Signal Accumulation Time (sec): Enter the time, in seconds, spent accumulating data into displayed channels.

Total Elapsed Time (sec): Enter the time, in seconds, to complete the acquisition of the spectral data. The total elapsed time includes the Signal Accumulation time (previous field), the settling time, and the overscan time.

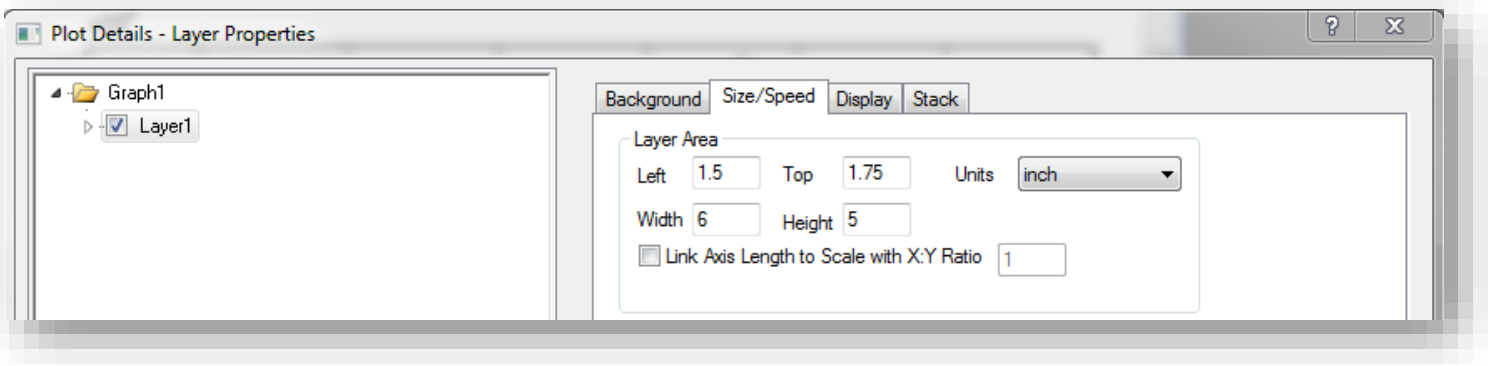
Number of Scans: Specify the number of times the signal for a given channel was counted.

Effective Detector Width (eV): Enter the detector width. For a multichannel detector, this would be the width, in eV, of the portion of the spectrum acquired simultaneously by the detector. (In a case where the effective width may vary with energy across the spectrum due to the type of analyzer used, an average detector width may be used, with the behavior described more fully in the 'Detector Description' in Section C.) For a single channel detector, the width can be listed as the eV/step in the spectral data.

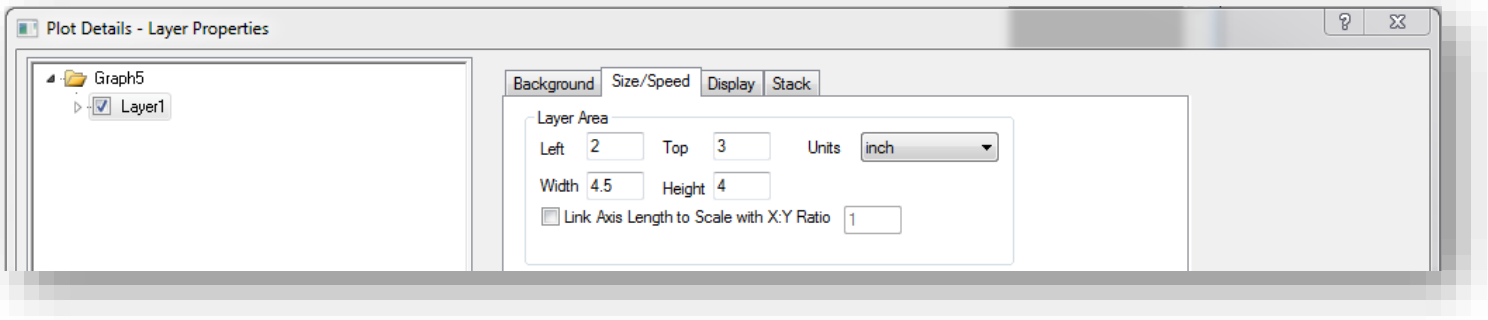
Appendix A- Origin Settings

Plot Details – Layer Properties - Size/Speed:

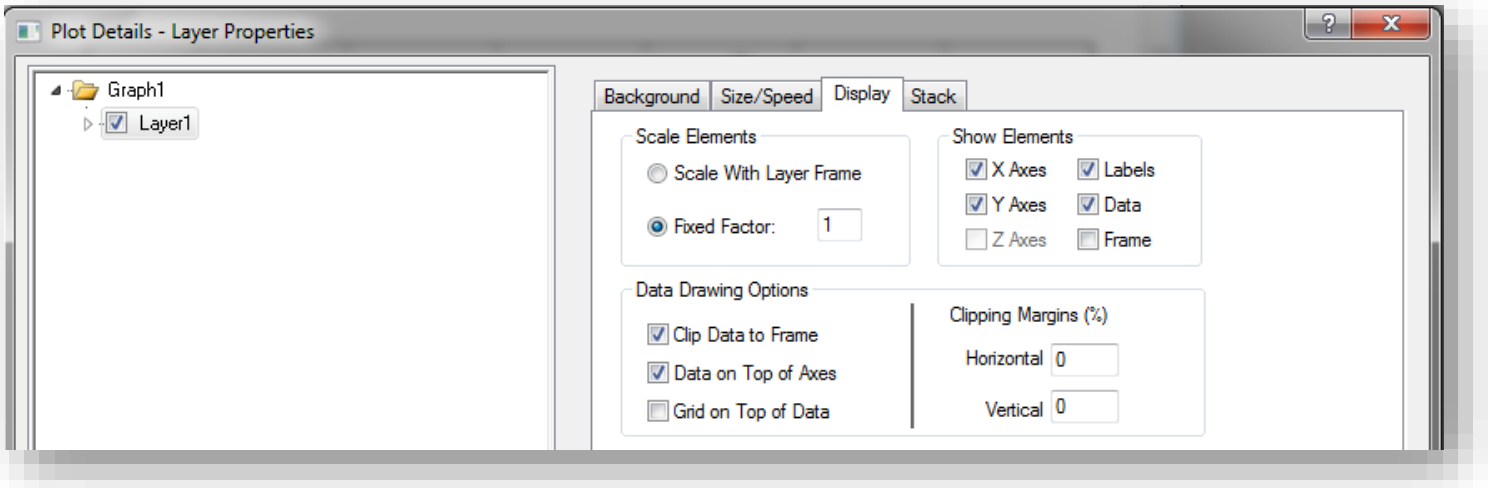
LEIS Spectrum



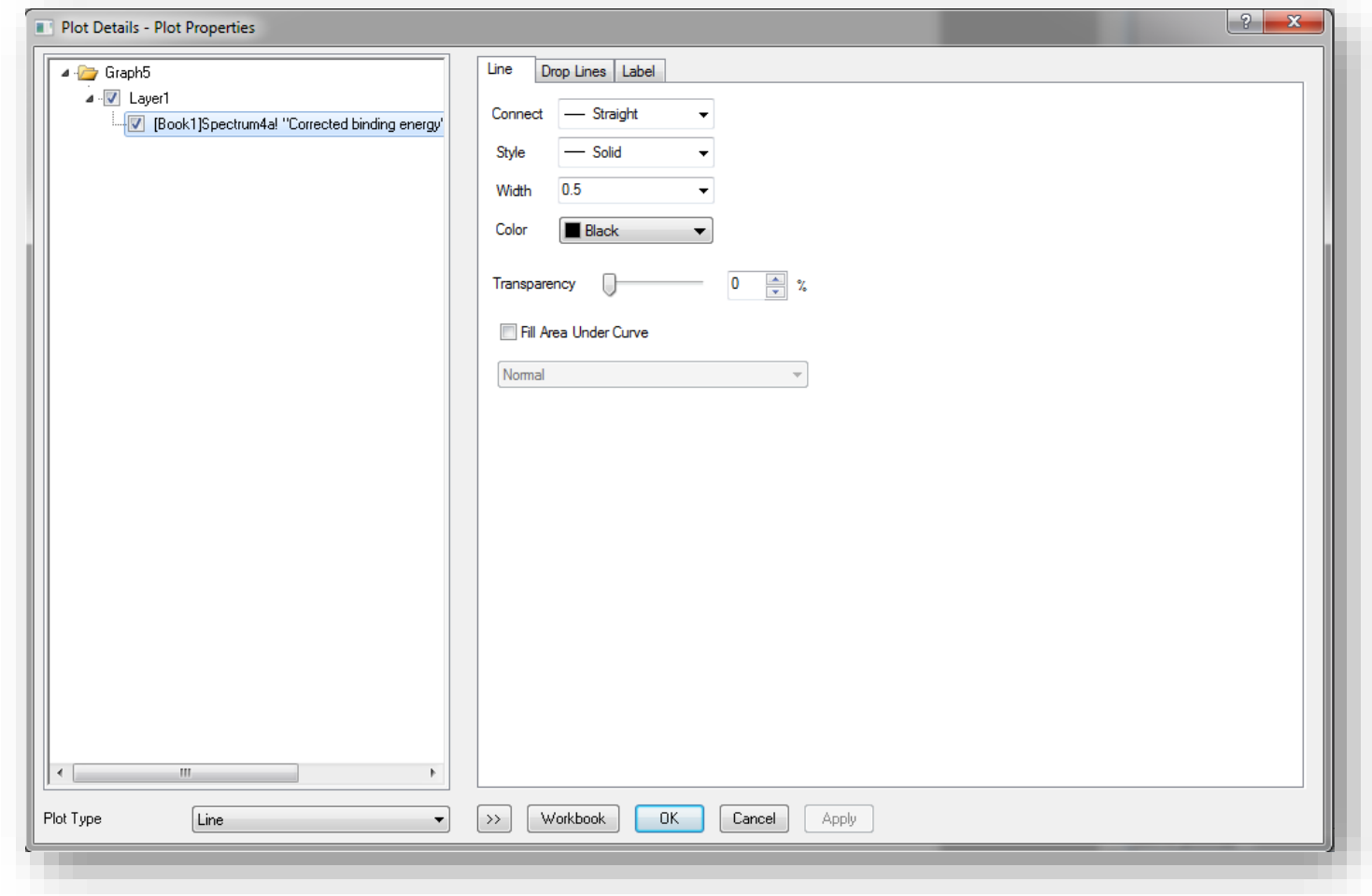
Calibration Spectrum



Plot Details – Layer Properties – Display (applies to both)

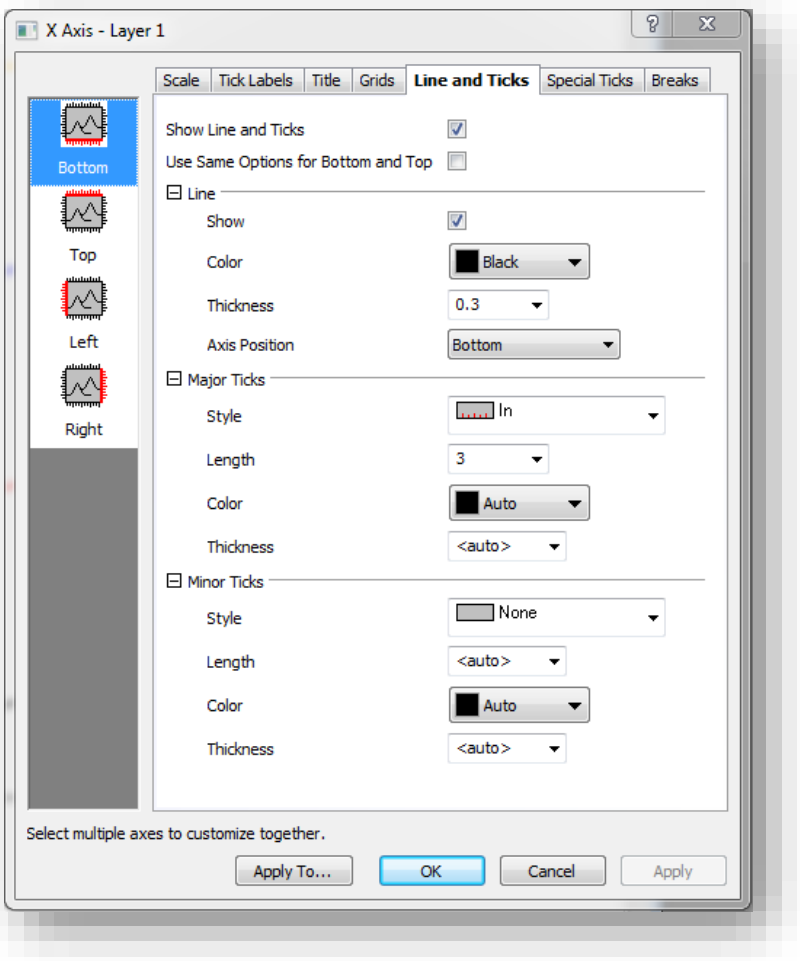


Plot Details – Plot Properties – Line (applies to both)



Note: For stacked spectra, authors may choose different colors for each spectrum.

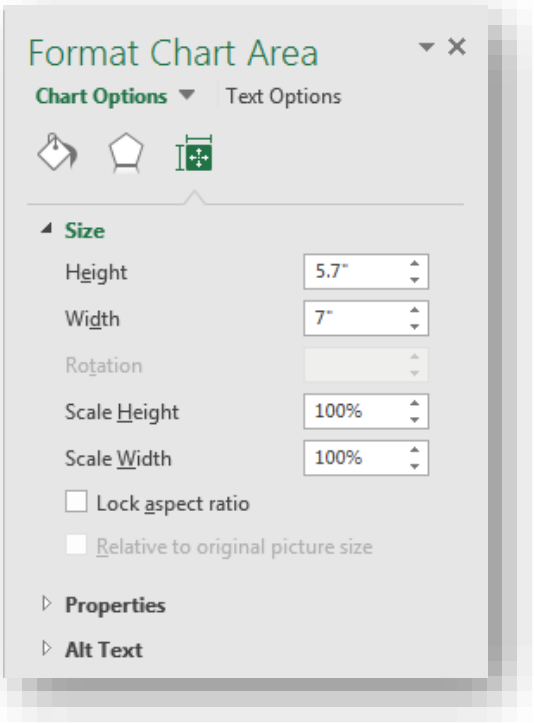
Axes - Line and Ticks (applies to all axes)



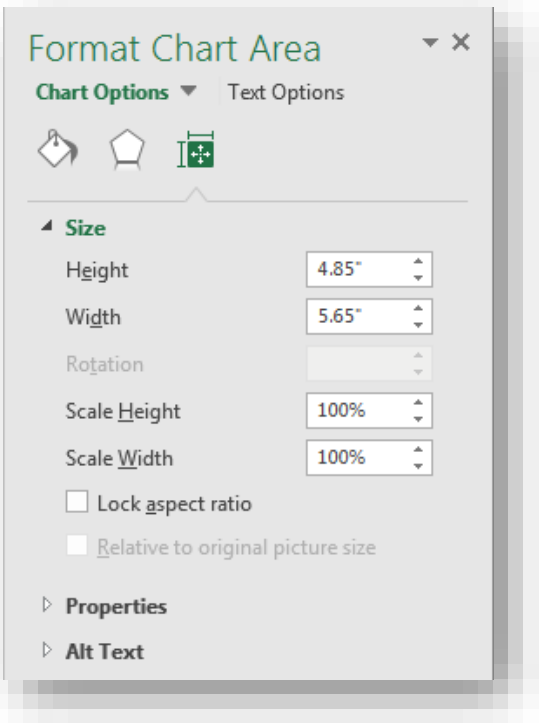
Appendix B- Excel Settings

Format Chart Area:

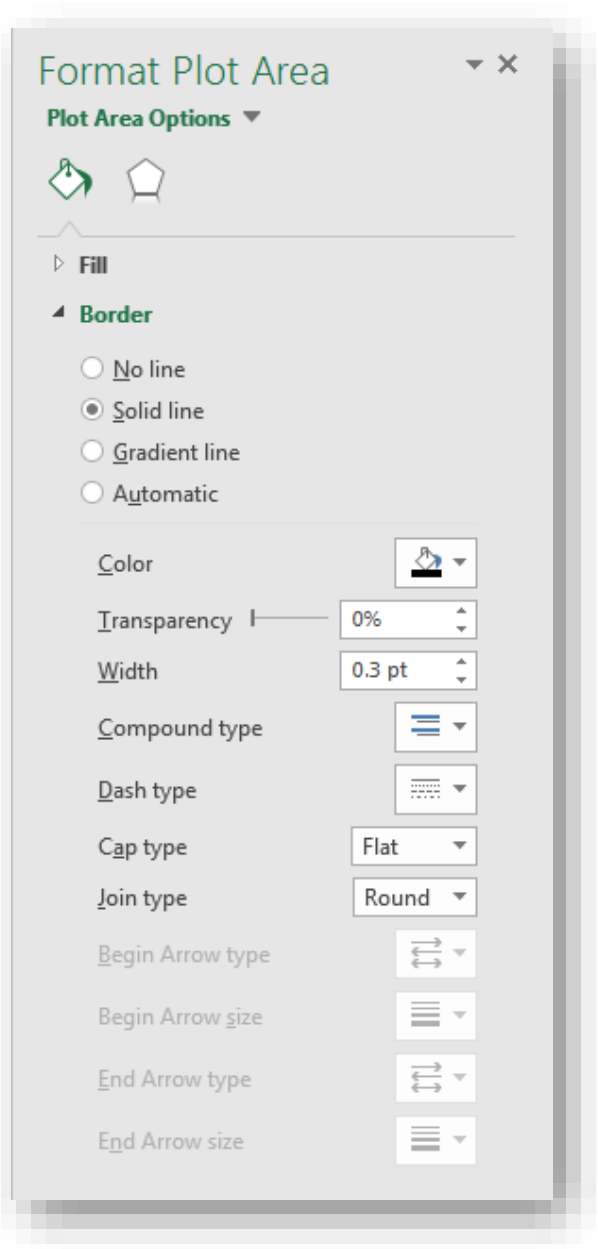
LEIS Spectrum



Calibration Spectrum

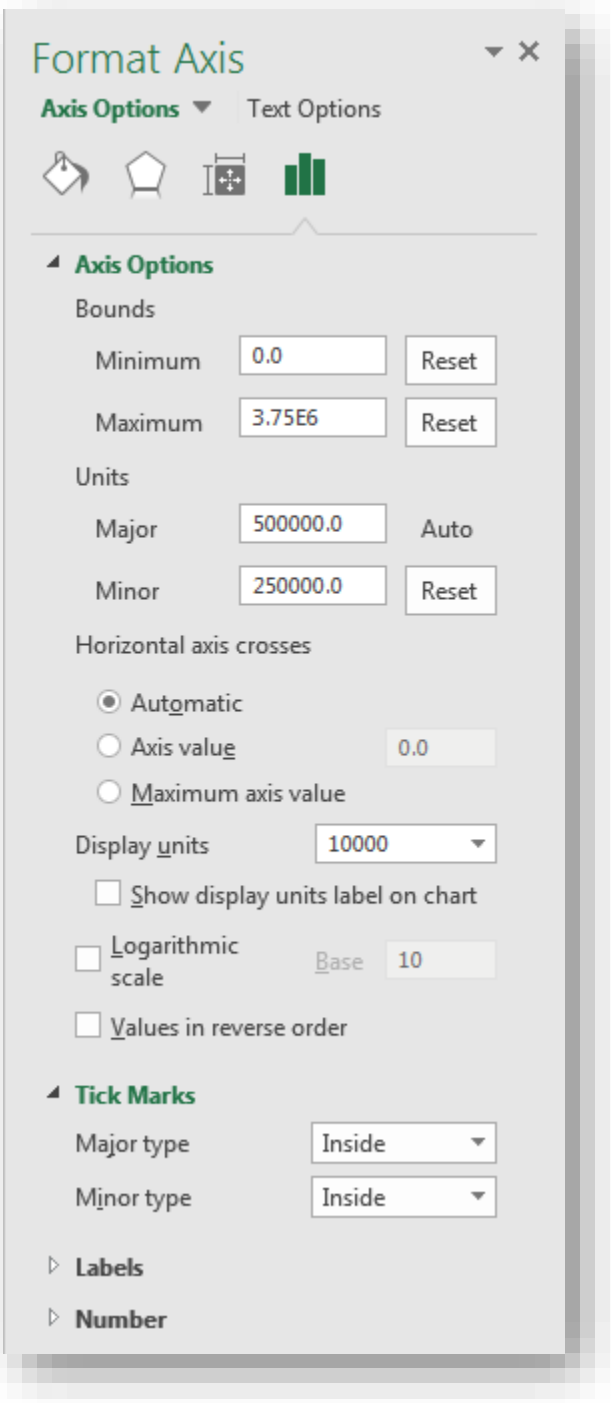


Format Plot Area (applies to both):



Note: plot area border color should be set to black.

Format Axes (applies to both):



Note: For Y-axis, adjust "Display units" so that axis values have no more than 3 significant figures. For both axes, set "Units Minor" value to be half of the "Units Major" value.

Format Data Series (applies to both):